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ABSTRACT SUBMISSION FORM

Evidence of a Jahn-Teller impurity in a cubic lattice displaying a compressed geometry

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Spontaneous symmetry-breaking around a defect site leads to interesting quantum phenomena, like tunnelling between various stable wells that, under the correct conditions could serve as the basis for applications like quantum computation[1,2]. Of particular interest is the Jahn-Teller distortion appearing in some transition-metal impurities in cubic lattices that usually involves the elongation of the metal ligand octahedron along one of its axes. For a long time it was believed that this was the case for a nickel-associated defect appearing in CaO:Ni^{2+} after irradiation[3], ascribed to a Ni^{3+} ($3d^7$) ion with a S=1/2 ground state[4]. First principle calculations together with an analysis of experimental data found for $3d^9$ and $3d^7$ ions in cubic oxides prove however that the centre found in irradiated CaO:Ni^{2+} corresponds to Ni^{+} under a static Jahn-Teller effect displaying a compressed equilibrium geometry[5]. To our knowledge this is the first genuine Jahn-Teller system (i.e. where exact degeneracy exists at the high-symmetry configuration) exhibiting compressed equilibrium geometry. Moreover, the present calculations[5] demonstrate that the anomalous positive $g_{\|}$-shift ($g_{\|} - g_0 = 0.065$) measured[3] at T = 20 K obeys to the superposition of $|3z^2\text{-}r^2\rangle$ and $|x^2\text{-}y^2\rangle$ states driven by quantum effects associated with the zero-point motion, a mechanism firstly put forward by O'Brien[6] and that, so far, had no rigorous experimental support. In the present case, that mechanism is shown to be enhanced by the low Jahn-Teller barrier (8.7meV) among equivalent configurations[5]. Finally an analysis of calculated energy barriers for different Jahn-Teller systems[2,5] allows us to explain the singular origin of the compressed geometry present in CaO:Ni^{+}.

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